arXiv:cond-mat/0612450v1 [cond-mat.mes-hall] 18 Dec 2006

Conductance oscillation and quantization in monoatomic Al wires

Ying Xu[1]‡, Xingqiang Shi[2], Zhi Zeng[2], Zhao Yang Zeng[1], and Baowen Li[3,4]

[1]Department of Physics, Jangxi Normal University, Nanchang 330022, China
[2]Key Laboratory of Material Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, Anhui 230031, China
[3] Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, 117542, Singapore
[4] NUS Graduate School for Integrative Sciences and Engineering, Singapore 117597, Singapore

Abstract.

We present first-principles calculations for the transport properties of monoatomic Al wires sandwiched between Al(100) electrodes. The conductance of the monoatomic Al wires oscillates with the number of the constituent atoms as a function of the wire length, either with a period of four-atom for wires with the typical interatomic spacing or a period of six-atom with the interatomic spacing of the bulk fcc aluminum, indicating a dependence of the period of conductance oscillation on the interatomic distance of the monoatomic Al wires.

PACS numbers: PACS 73.63.Rt; 73.23.Ad

1. Introduction

Atomic wires, which can be produced by means of either scanning tunnelling microscope[1], mechanically controllable break junction techniques[2], or transmission electron microscope[3], have attracted increasing attentions both theoretically and experimentally [4]. For monovalent atomic wires, the even-odd oscillations of the wire conductance with the wire length has been analyzed explicitly and demonstrated numerically[5], and perfect transmission is found for atom chains of an odd number atoms and a smaller transmission in the even number case. The even-odd oscillations of conductance has been confirmed experimentally for atomic wires formed by noble-metal Au, Pt and Ir atoms[6]. An anomalous oscillation of conductance is found for atomic chains composed of alkali-metal atoms (such as Na, Cs) [7-9], with perfect transmission in the case of even number. However, for polyvalent atomic wires such as Pb and Al,

‡ yingxu@jxnu.edu.cn

multiple conductance channels contribute to the conductance, the situation becomes more complicated, and more interesting phenomena are expected.

The transport properties of monoatomic wires formed by Al atoms have been studied with the first-principles method by several groups[10-12]. Lang has investigated the resistance of Al atomic wires connecting two semi-infinite metallic electrodes[10]. Kobayashi et al.[11] has studied the conducting channels for monoatomic Al wires by the recursion-transfer matrix method. They reveal that three open channels can contribute to the current through the Al atomic wire, and channel transmission are sensitive to the geometry of the wire. Ono and Hirose [12] have studied the electronic conductance of a three-Al-atom suspended between genuine semi-infinite aluminum crystalline electrodes. They have demonstrated that just one conducting channel is widely open at the Fermi level. However, we notice that, in the above calculations, the interatomic spacing between Al atoms is assumed to be the same as the bulk fcc one. The influence of the electrode model structure on the sandwiched wire has been clarified by Fujimoto et al.[13]. Conductance oscillations with a period of four-atom have been shown by Thygesen and Jocobsen with the help of the plane-wave based pseudopotential code for the Al wire between two Al(111) electrodes[14]. The interatomic spacing of the wire is set to be 2.39 Å, the typical interatomic distance of the Al wires.

In the present paper, we perform a first-principles calculations on the conductance of the monoatomic Al wires attached to a pair of Al(100) bulk electrodes so as to clarify the effect of the interatomic spacing of the wire. Our results are consistent with that obtained in ref. [14], when a smaller interatomic atomic spacing (the typical interatomic distance of Al wires) is used. While if we choose the interatomic distance of the bulk fcc aluminum, the six-atom period of the conductance oscillation is observed, which is different from the former case. Our results suggest that the period of conductance oscillation depends on the interatomic spacing of the wire.

2. Methodology

The calculations have been performed by using a recently developed first-principles package TranSIESTA-C[15-17]. The package is based on the combination of density function theory (DFT) implemented in the well tested SIESTA method with the nonequilibrium Green function technique. TranSIESTA-C is capable of modelling self-consistently the electrical properties of nanoscale devices that consist of an atomic scale system coupled to two semi-infinite electrodes. The system considered can be divided into three parts: the left electrode, the scattering region and the right electrode. The central region also consists of two layers of surface atoms at left and three layers of surface atoms at right in order to include the interaction between the electrode and the atomic wire. The end of Al atomic wire is fixed at the hollow sites of the Al(100). The distance between the end atom of the wire and the electrode edge is set to be 1 Å. In our calculations two values of interatomic spacing of the wire are used, one is 2.86 Å, the same distance as in the bulk fcc aluminum; the other is 2.39 Å, typical Al-Al

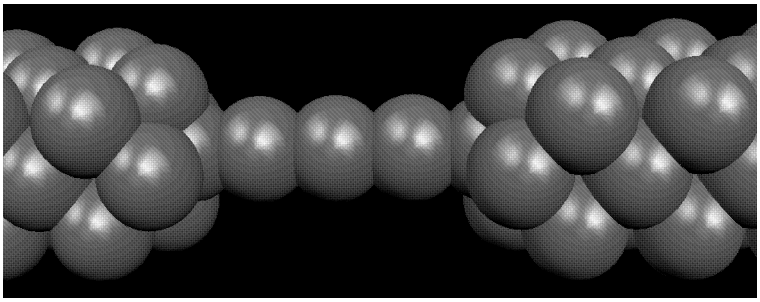

Figure 1. A schematic representation of an aluminum atom chain with 5 Al atoms sandwiched between a pair of Al(100) electrodes.

atom spacing. The z-direction is set to be parallel to the wire axis. Figure 1 shows the system we considered: a monoatomic Al wire is sandwiched between a pair of Al(100) electrodes.

3. Results and discussions

We first calculate the conductance of the monoatomic Al wire with the typical interatomic spacing 2.39 Å, as a function of the number of the constituent aluminum atoms. The results are shown Fig. 2 (a). The figure clear shows an oscillation with a period of four-atom which is similar to that one found in Ref. [14]. However, it

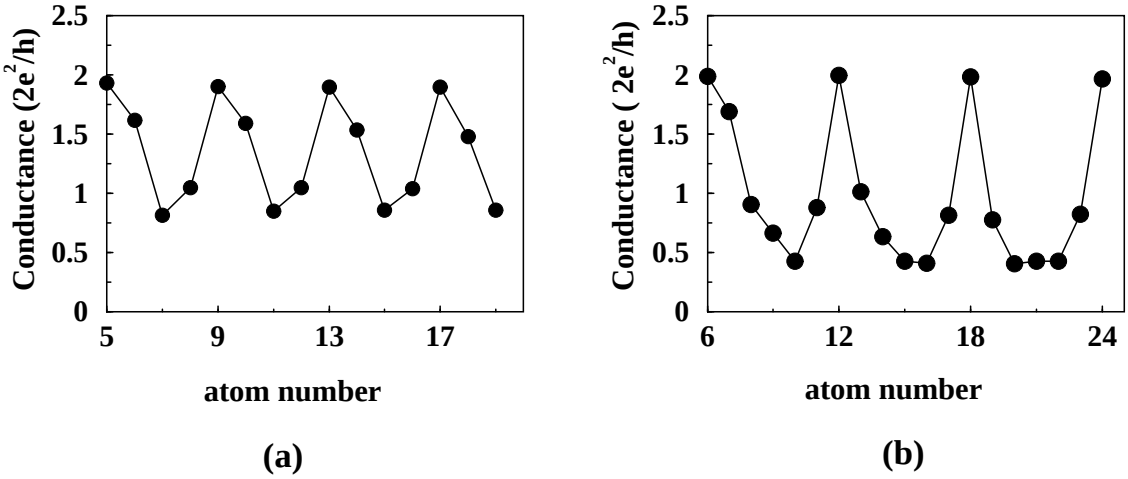

Figure 2. Conductance of monoatomic Al wires connecting to a pair of Al(100) electrode as a function of the number of Al atoms. (a) Al interatomic spacing is 2.39 Å(b) The interatomic spacing is 2.86 Å which is the same as that of the bulk fcc aluminum.

is worthwhile to point out that in our calculations, the equilibrium conductance of the system varies between $0.8 \sim 1.9$ G_0 (G_0=$2e^2/h$), and the maximal conductance occurs as the number of wire atoms takes values 5, 9, 13 $\cdots$. While in ref. [14], the maximal values of the conductance correspond to the atom number 3, 7, 11 $\cdots$. and the conductance range is $0.5 \sim 1.7$ G_0. The different phase and amplitude of the conductance oscillations may originate from the geometrical structure difference of the electrodes. We use a pair of semi-infinite Al(100) electrodes while Thygesen and Jocobsen [14] use two Al(111) electrodes.

One may ask, if the monoatomic Al chain is elongated, namely, the spacing between Al atoms is increased, can one expect the same four-atom period for the conductance as a function of the number of Al atoms? To answer this question, we calculate the conductance of Al atom wires coupled to the same pair of Al(100) electrodes as the number of the Al atoms forming the chains, as the spacing of the chains is chosen the same as the interatomic spacing of the bulk fcc aluminum 2.86 Å. The results are shown in Figure 2 (b). To our surprise, the conductance exhibits oscillations with a period of six-atom. Such an observation suggests that the period of the conductance oscillations of monoatomic Al wires is related to the interatomic spacing of the wires.

To confirm our observation of the conductance oscillation with a period of four-

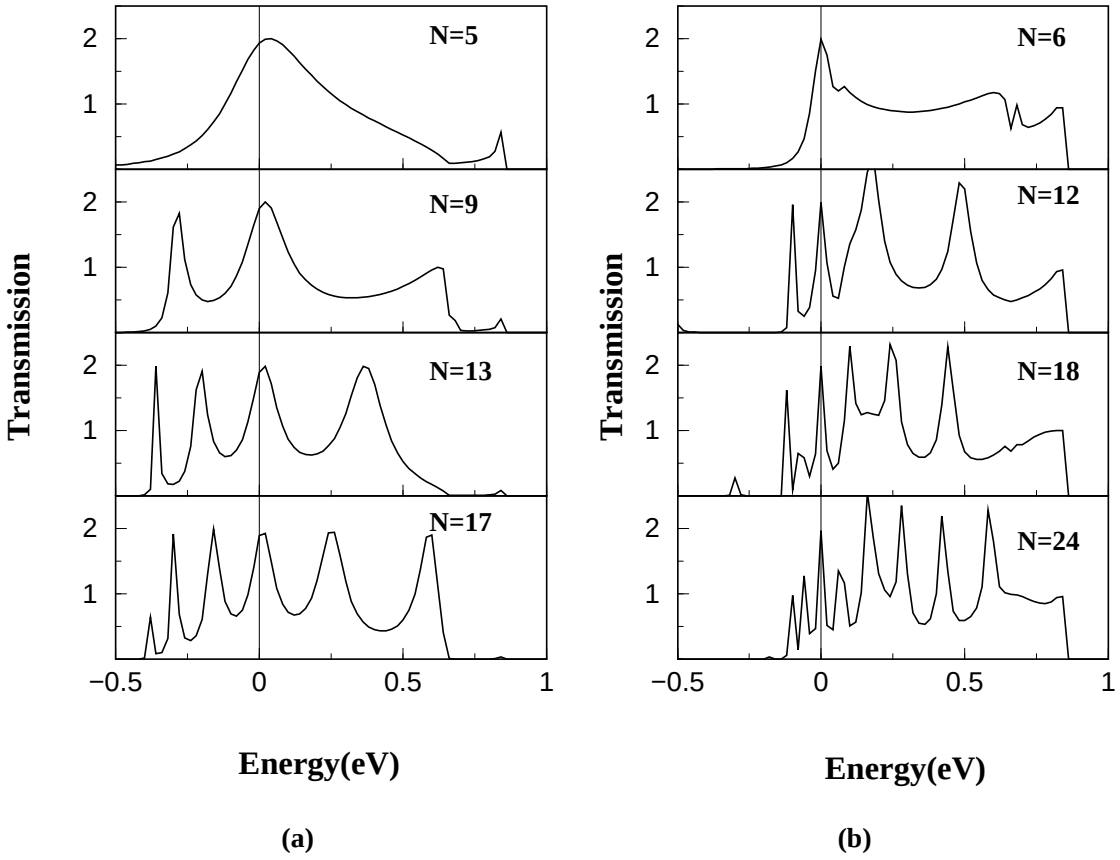

Figure 3. Transmission spectra for monoatomic Al wires for different number of constituent Al atoms. (a) With the typical interatomic spacing of Al 2.39 Å(b) With the interatomic spacing of the bulk fcc aluminum 2.86 Å .

atom or six-atom for the monoatomic Al wire with different interatomic spacings sandwiched between a pair of Al(100) electrodes, we also calculate the transmission spectra of the system and show the results in Fig. 3. One can see a clear level splitting as the increase of the number of the resonant peaks with increase of the number of the constituent Al atoms. This can be easily tested from an analysis of the Molecular Projected Self-consistent Hamiltonian (MPSH). The eigenstates of MPSH are in fact the molecular orbitals renormalized by the molecule-electrode couplings. As an example, one would expect 12 eigen levels for the wire containing 12 monovalent atoms. According the Landauer-B*ü*ttiker theory, the equilibrium conductance is proportional to the transmission probability at the Fermi level. Therefore the conductance oscillations of monoatomic Al wires are equivalent to the coincidence of transmission peaks at the Fermi level for some specific numbers of the Al atoms forming the wire. From Figs. 3 (a) and (b), one clearly sees such a coincidence of transmission peaks as the number of the Al atoms is 5, 9, 13, 17 for the wire with the interatomic distance of the bulk fcc aluminum, and 6, 12,18,24 for the wire with the typical interatomic distance of Al.

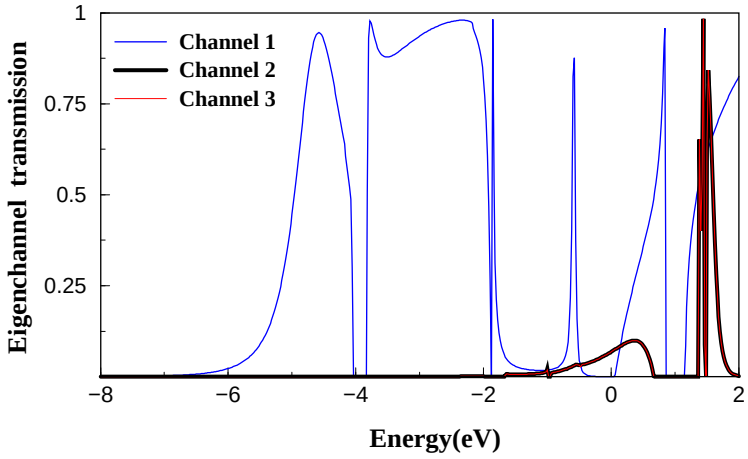

Figure 4. Eigenchannel transmission spectra of the σ channel (channel 1) and the two degenerate π transmission eigenchannels (channel 2 and 3) for the three-Al-atom wire with the interatomic spacing of the bulk fcc aluminum attached to a pair of Al (100) electrodes.

The eigenchannel decomposition of transmission spectra provides some useful information about transport properties of two-probe systems. Therefore, we look at the transmission spectra of a three-Al-atom wire with the interatomic spacing of the bulk fcc aluminum 2.86 ÅThe eigenchannel transmission spectra is shown in Figure 4. We note that the transmission spectra in this work are different from the previous results for the three-Al-atom wire based on various types of jellium electrode models. It confirms that the conductance of Al atomic wires is dependent on the detailed geometric structure of the electrodes[13].

It is well known that, the valence electron configuration of Al atom is $3s^2 3p^1$. The s and p_z orbitals constitute σ-character channel and p_x, p_y orbitals constitute degenerate π-character channels, as clearly shown in Fig. 4. The σ channel contributes nothing to current and thus the equilibrium conductance, because Fig. 4 tells us that the transmission of the σ channel at the Fermi level is zero. Two degenerate π channels contribute a small amount to the equilibrium conductance of the three-Al-atom wire, since the transmission probabilities of these two degenerate π channels are the same, of the value of about 0.07. We also calculate the eigenchannel transmission spectra for the monoatomic Al wire with different numbers of the constituent atoms. We find that for the Al wires containing 6, 12, 18 Al atoms, two degenerate π channels contribute mainly to the equilibrium conductance, each contribution to conductance being about one conductance quanta one G_0; and the contribution from the σ channel is still zero. Such a conductance quantization is suggested as a result of charge neutrality and resonant character of the sharp tip structure of the wire-electrode contacts[18].

To explain the six-atom period of the conductance oscillation of monoatomic Al

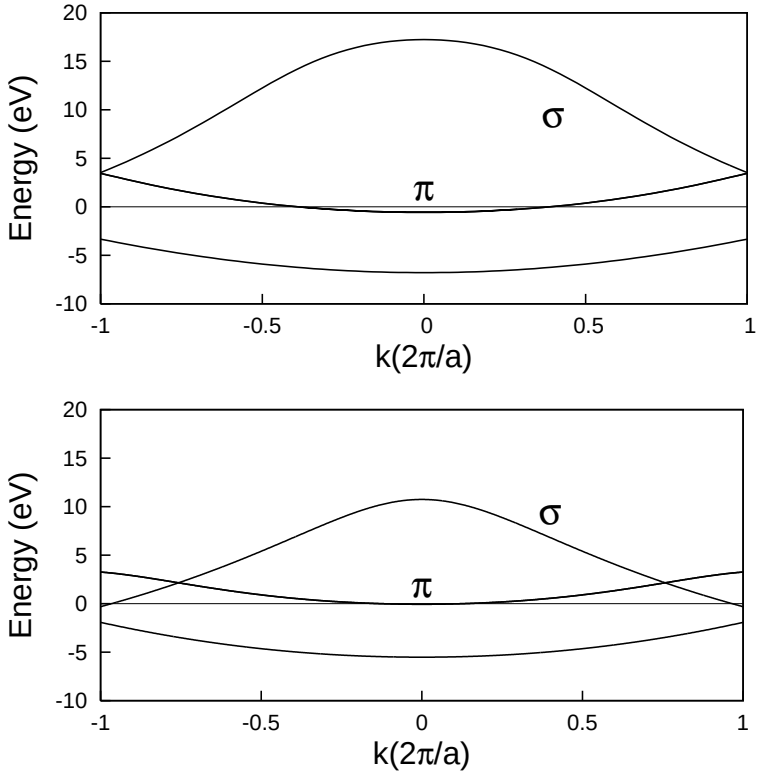

Figure 5. The energy band structure of infinite Al wires with the typical interatomic distance 2.39 Å (upper panel) and the interatomic distance of the bulk fcc aluminum 2.86 Å (lower panel)

wires with the interatomic spacing of the bulk fcc aluminum, we perform band structure calculations for an infinite Al wire with the typical interatomic distance 2.39 Å and the interatomic distance of the bulk fcc aluminum 2.86 Å attached to a pair of Al(100) electrodes. The results are shown in Figure 5. The period of conductance oscillations is determined by the filling factor of the conducting bands with the consideration of local charge neutrality[14]: the filling factor is the inverse of the period of the conductance oscillation. Comparing the band structures of the infinite Al wire with the typical interatomic spacing and with the the interatomic spacing of the bulk fcc aluminum, we find that the valence band - the bonding σ band, formed by the σ orbitals of Al atoms, is fully filled in both cases. For the infinite Al wires with the typical interatomic spacing, the conducting band is formed by the degenerate π orbitals, while the conducting band includes the contributions of both the anti-bonding σ band and the degenerate π band

for the monoatomic Al wires with the interatomic distance of bulk fcc aluminum. Such a dependence of the energy band structure of an infinite Al wire on the interatomic distance may be associated with the Pierce distortion effect, and is similar to the findings by Okano et al.[19]. It is known that each Al atom provides three electrons with two occupying the bonding σ valence band and another occupying the conducting band. Therefore one finds, for an infinite monoatomic Al wires, a filling factor 1/4 with the typical interatomic distance and a filling factor 1/6 with the interatomic distance of the bulk fcc aluminum. It is such a filling factor imposed by local charge neutrality that causes the conductance oscillation with a period of either four-atom or six-atom, depending on the interatomic distance of Al atoms forming the wire. However, it is difficult to determine the phase of the conductance oscillations of the monoatomic Al wires, due to the limitations of the soft package TranSIESTA-C we have used.

4. Conclusion

In conclusion, we have investigated conductance oscillations of a monoatomic Al wires with different interatomic spacings sandwiched between a pair of Al (100) electrodes with a well-developed soft package TranSIESTA-C. Conductance oscillations with a period of four-atom and six-atom are observed for the monoatomic wire with the typical interatomic distance and the interatomic distance of the bulk fcc aluminum. The period of the conductance oscillations is determined by the filling factor of the conducting band of Al wires with specific interatomic spacing.

5. Acknowledgements

This work was supported by the National Natural Science Foundation of China under Grant No. 10404010, the Project-sponsored by SRF for ROCS, SEM, the Foundation of Jiangxi Educational Committee under Grant No. 112[2006], and the Talent Fund of Jiangxi Normal University under Grant No. 1186 and 1187. BL was supported in part by a FRG grant of NUS.

[1] A. Dhirani, P.-H. Lin *et al*, J. Chem. Phys. **106**, 5249 (1997).
[2] M. A. Reed *et al*, Science **278**, 252 (1997).
[3] H. Ohnishi, Y. Kondo, and K. Takayanagi, Nature (London) 395, 780 (1998).
[4] N. Agraït, A. L. Yeyati, and J. M. van Ruitenbeek, Phys. Rep. 377, **81** (2003).
[5] Z. Y. Zeng and F. Claro, Phys. Rev. B **65**, 193405 (2002); H. -S. Sim, H. -W. Lee, K. J. Chang, Phys. Rev. Lett.**87**, 096803 (2001).
[6] R. H. M. Smit, C. Untiedt, G. Rubio-Bollinger, R. C. Segers and J. M. van Ruitenbeek, Phys. Rev. Lett. **91**, 076805 (2003).
[7] N. D. Lang, Phys. Rev. Lett. **79**, 1357 (1997).
[8] P. Havu, T. Torsti, M. J. Puska, and R.M. Nieminen, Phys. Rev. B **66**, 075401 (2002).
[9] Y. Asai and H. Fukuyama, Phys. Rev. B **72**, 085431 (2005).
[10] N. D. Lang, Phys. Rev. B, **52**, 5335 (1995).
[11] N. Kobayashi, M. Brandbyge, and M. Tsukada, Phys. Rev. B **62**, 8430 (2000).

[12] T. Ono and K. Hirose, Phys. Rev. B **70**, 033403 (2004).
[13] Y. Fujimoto, Y. Asari, and H. Kondo, Phy. Rev. B **72**, 113407 (2005).
[14] K. S. Thygesen and K.W. Jacobsen, Phys. Rev. Lett. **91**, 146801 (2003).
[15] M. Brandbyge, J. -L. Mozos, P. Ordejón, J. Taylor, and K. Stokbro, Phys. Rev. B **65**, 165401 (2002).
[16] J. Taylor, H. Guo, and J. Wang, Phys. Rev. B **63**, 245407 (2001).
[17] José M. Soler *et. al*, J. Phys.: Condens. Matter **14**, 2745 (2002).
[18] A. Levy Yeyati, A. Martín-Rodero, and F. Flores, Phys. Rev. B **56**, 10369 (1997).
[19] S. Okano, K. Shiraishi, and A. Oshiyama, Phys. Rev. B **69**, 045401 (2004).